

ON THE CONNECTION BETWEEN THE LIOUVILLE EQUATION AND THE SCHRÖDINGER EQUATION

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Abstract

We derive a classical Schrödinger type equation from the phase space Liouville equation valid for an arbitrary nonlinear potential $V(x)$. The derivation is based on a Wigner type Fourier transform of the classical phase space probability distribution, which depends on a small constant α with dimension of action, that will be characteristic of the microscopic phenomena. In order to obtain the Schrödinger type equation, two requirements are necessary: 1) It is assumed that the appropriately defined classical probability amplitude $\Psi(x, t)$ can be expanded in a complete set of functions $\Phi_n(x)$ defined in the configuration space; 2) the classical phase space distribution $W(x, p, t)$ obeys the Liouville equation and is a real function of the position, the momentum and the time.

We show that for α equal to the Planck's constant \hbar , the evolution equation for the *classical* probability amplitude $\Psi(x, t)$ is identical to the Schrödinger equation. The wave particle duality principle, however, is not introduced in our paper.

Key words: Foundations of quantum mechanics; Wigner phase-space distributions; Quantum electrodynamics; Vacuum fluctuations; Stochastic electrodynamics

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1 Introduction

In 1932 E. Wigner published an important paper [1, 2] where he introduced what is called today *the Wigner's quasi probability function*, or simply *Wigner's phase space function*. We shall denote it by $Q(x, p, t)$ and it is connected with the Schrödinger wave equation solutions $\psi(x, t)$ by the expression:

$$Q(x, p, t) = \frac{1}{\pi\hbar} \int \psi^*(x - y, t) \psi(x + y, t) e^{-\frac{2ipy}{\hbar}} dy, \quad (1)$$

where \hbar is the Planck's constant. We recall that Wigner's intention was to obtain a quantum mechanical description of the classical phase space phenomena.

It was stated later, by Wigner and O'Connell [3], that the definition (1) is the only one that satisfies a set of conditions that are expected on physical grounds.

Notice, however, that the Planck's constant \hbar enters in the above expression in a combination that was not completely clarified by Wigner and other authors [1-7]. We know that the Planck's constant \hbar is related to the *electromagnetic fluctuation phenomena* characteristic of Quantum Electrodynamics [8] and Classical Stochastic Electrodynamics [9-12]. However, for simplicity, these electromagnetic fluctuations will be not considered in our paper.

We would like to mention that, if applied to an arbitrary solution $\psi(x, t)$ of the Schrödinger wave equation, the expression (1) may lead to *negative*, or even *complex*, phase space probability densities, suggesting that many solutions of the Schrödinger wave equation cannot be associated with genuine phase space probability distributions, that is, the relation (1) is problematic. Simple examples are the excited states of the harmonic oscillator [9]. Here, following França and Marshall [9], we shall consider that these excited states are simply useful mathematical functions. We shall clarify this point later.

It is also well known [1, 6] that $Q(x, p, t)$ defined in (1) propagates in time according to the quantum Liouville equation

$$\frac{\partial Q}{\partial t} = -\frac{p}{M} \frac{\partial Q}{\partial x} + \frac{\partial V}{\partial x} \frac{\partial Q}{\partial p} + \frac{\left(\frac{\hbar}{2i}\right)^2}{3!} \frac{\partial^3 V}{\partial x^3} \frac{\partial^3 Q}{\partial p^3} + \frac{\left(\frac{\hbar}{2i}\right)^4}{5!} \frac{\partial^5 V}{\partial x^5} \frac{\partial^5 Q}{\partial p^5} + \dots, \quad (2)$$

provided that $\psi(x, t)$ satisfies the Schrödinger wave equation. Here $F(x) = -\partial V/\partial x$ is the arbitrary nonlinear force acting on the particle with mass M .

The equation (2) shows that the definition (1), and the Schrödinger equation, do not lead to the classical Liouville equation. We recall that, according to the correspondence principle, one should necessarily obtain the Liouville equation if the mass M is large enough. Therefore, the relationship between the equation (1), the Schrödinger equation and the Liouville equation is also problematic.

In our paper, starting with the classical Liouville equation, we shall see the mathematical and the physical conditions to connect it with an equation which is formally identical to the Schrödinger equation for a *classical* probability amplitude $\Psi(x, t)$ defined in the configuration space.

By means of the theorem established within the section 2, we show that the connection between the Liouville equation and the Schrödinger type equation is valid for an arbitrary potential $V(x)$. This connection was presented in reference [4], restricted to the case where the potential $V(x)$ is quadratic in the variable x .

Our presentation is organized as follows. We give, within section 2, the mathematical background necessary to connect the classical phase space probability distribution to the classical configuration space probability amplitude $\Psi(x, t)$. For clarity sake, we shall denote $\psi(x, t)$ a solution of the Schrödinger wave equation and $\Psi(x, t)$ the classical probability amplitude. The direct relation between the Liouville equation for an arbitrary potential $V(x)$, and the classical Schrödinger type equation is presented within section 3. A brief discussion and our conclusions are presented in the final section.

2 Mathematical background

Our starting point is the Liouville equation for the probability distribution in phase space, denoted by $W(x, p, t)$. The Liouville equation is such that

$$\frac{\partial W}{\partial t} + \frac{p}{M} \frac{\partial W}{\partial x} + F(x) \frac{\partial W}{\partial p} = 0. \quad (3)$$

The nonlinear force acting on the particle with mass M will be denoted by $F(x) = -\partial V(x)/\partial x$ and $V(x)$ is an arbitrary continuous function. The solutions of the equation (3) are obtained in conjunction with the solutions of the Newton equation

$$M \frac{d^2 x}{dt^2} = F(x), \quad (4)$$

and the classical positive distribution function, $W_0(x_0, p_0)$, associated with the initial conditions x_0 and p_0 , namely

$$W(x, p, t) = \int dx_0 \int dp_0 W_0(x_0, p_0) \delta(x - x_c(t)) \delta(p - p_c(t)). \quad (5)$$

Here $x_c(t)$ is the classical trajectory and $p_c(t) = m\dot{x}_c(t)$. Notice that $x_c(t)$, and $p_c(t)$, depend on x_0 and p_0 . Therefore, $W(x, p, t)$ is always real and positive, and the classical probability amplitude $\Psi(x, t)$ is such that

$$|\Psi(x, t)|^2 = \int_{-\infty}^{\infty} dp W(x, p, t). \quad (6)$$

The above definition is not enough to determine the complex amplitude $\Psi(x, t)$. To achieve this goal we shall use the Liouville equation (3).

The Liouville equation for $W(x, p, t)$ has a close relation with a classical Schrödinger type equation for $\Psi(x, t)$, as we shall see in the next section. In order to clearly explain this relationship we shall establish a useful theorem based on a convenient Fourier transform of $W(x, p, t)$ similar to that used in equation (1).

Theorem:

Consider the Fourier transform defined by

$$T[W](x, y, t) = \int_{-\infty}^{\infty} W(x, p, t) e^{\frac{2ipy}{\alpha}} dp, \quad (7)$$

where α is a *small* constant with dimension of action. The mathematical definition (7) has a physical meaning only when $y \approx 0$ because in this case, the equation (7) becomes identical to (6) and gives us the probability distribution in the configuration space. Mathematically, we can write $T[W](x, y = 0, t) = |\Psi(x, t)|^2$. We shall show that $T[W](x, y, t)$ can always be expressed in the form

$$T[W](x, y, t) = \Psi^*(x - y, t) \Psi(x + y, t), \quad (8)$$

provided that $W(x, p, t)$ is a *real function* of its variables.

Proof:

Consider any set of functions $\Phi_n(x)$, that satisfy the completeness relation

$$\sum_n \Phi_n^*(x) \Phi_n(y) = \delta(x - y), \quad (9)$$

and are orthogonal to each other. An example of these functions is the set

$$\Phi_n(x) = \frac{1}{\sqrt{2b}} e^{\frac{in\pi x}{b}}, \quad (10)$$

where $n = 0, \pm 1, \pm 2, \pm 3, \dots$ and b is a positive constant ($-b < x < b$). Other sets of functions $\Phi_n(x)$ can be used without loss of generality [2, 9].

Therefore, any complex probability amplitude $\Psi(x, t)$ can be expressed as

$$\Psi(x, t) = \sum_n a_n(t) \Phi_n(x), \quad (11)$$

where $a_n(t)$ are the coefficients of the expansion. Different sets of coefficients $a_n(t)$ will give different probability amplitudes $\Psi(x, t)$. One can show, from the orthogonality properties of the functions $\Phi_n(x)$, that

$$a_n(0) = \int dx \Phi_n^*(x) \Psi(x, 0). \quad (12)$$

Let $W_{mn}(x, p)$ be phase-space functions defined by [2, 9]

$$W_{mn}(x, p) = \frac{1}{\pi\alpha} \int dy \Phi_m^*(x - y) \Phi_n(x + y) e^{-\frac{2ipy}{\alpha}}, \quad (13)$$

where α is the same constant introduced in (7). This is a convenient mathematical definition because the functions $W_{mn}(x, p)$ have useful properties as we shall see in what follows. Notice that the functions $W_{mn}(x, p)$ can be *positive, negative or even complex functions* [2, 9].

The functions $W_{mn}(x, p)$ constitute a complete and orthogonal set of functions in phase space. The completeness can be verified as follows:

$$\begin{aligned} & \sum_m \sum_n W_{mn}^*(x, p) W_{mn}(y, q) = \\ &= \frac{1}{(\pi\alpha)^2} \int d\xi \int d\eta e^{-\frac{2i}{\alpha}(q\eta - p\xi)} \sum_m \Phi_m(x - \xi) \Phi_m^*(y - \eta) \sum_n \Phi_n(y + \eta) \Phi_n^*(x + \xi) \\ &= \frac{1}{\pi\alpha} \delta(x - y) \delta(q - p). \end{aligned} \quad (14)$$

In the last equality the fact that functions $\Phi_n(x)$ form a complete set was used, and we also used the Fourier integral representation for the Dirac's delta function.

A verification of the orthogonality requirement can be obtained in an analogous way and leads us to the following relation [2, 9]:

$$\int dx \int dp W_{mn}^*(x, p) W_{rs}(x, p) = \frac{1}{\pi\alpha} \delta_{mr} \delta_{ns}. \quad (15)$$

Therefore, it is always possible to put the classical phase-space distribution $W(x, p, t)$ in the form

$$W(x, p, t) = \sum_m \sum_n C_{mn}(t) W_{mn}(x, p), \quad (16)$$

where the coefficients $C_{mn}(t)$ are only functions of the time t [9].

By substituting the explicit form of $W_{mn}(x, p)$ in the last equation, we obtain the formal expression

$$W(x, p, t) = \frac{1}{\pi\alpha} \int dy \sum_m \sum_n C_{mn}(t) \Phi_m^*(x - y) \Phi_n(x + y) e^{-\frac{2ipy}{\alpha}}. \quad (17)$$

Since $W(x, p, t)$ is a *real* function we have

$$W(x, p, t) = W^*(x, p, t). \quad (18)$$

Using the relation (18) we get the following equality:

$$\begin{aligned} \int dy \sum_m \sum_n C_{mn}(t) \Phi_m^*(x - y) \Phi_n(x + y) e^{-\frac{2ipy}{\alpha}} &= \\ = \int dy \sum_m \sum_n C_{mn}^*(t) \Phi_m(x - y) \Phi_n^*(x + y) e^{\frac{2ipy}{\alpha}}. \end{aligned} \quad (19)$$

Considering the change of variables $y = -\xi$, and exchanging the dummy indices m and n , we can write (19) in the form

$$\begin{aligned} \int dy \sum_m \sum_n C_{mn}(t) \Phi_m^*(x - y) \Phi_n(x + y) e^{-\frac{2ipy}{\alpha}} &= \\ = \int d\xi \sum_m \sum_n C_{nm}^*(t) \Phi_m^*(x - \xi) \Phi_n(x + \xi) e^{-\frac{2ip\xi}{\alpha}}. \end{aligned} \quad (20)$$

From this equation we conclude that

$$C_{mn}(t) = C_{nm}^*(t). \quad (21)$$

Therefore, the elements $C_{mn}(t)$ can be written in the following form:

$$C_{mn}(t) = a_m^*(t)a_n(t), \quad (22)$$

where the functions $a_n(t)$ are only functions of the time t [9]. In order to make the connection with the probability amplitude $\Psi(x, t)$ we shall assume that the functions $a_n(t)$ are the same functions introduced above in the equation (11).

Using (22), (17) and (7) we obtain

$$\begin{aligned} & \int dp W(x, p, t) e^{\frac{2ipy}{\alpha}} = \\ &= \frac{1}{\pi\alpha} \int dy' \left[\sum_m a_m^*(t) \Phi_m^*(x - y') \right] \left[\sum_n a_n(t) \Phi_n(x + y') \right] \int dp e^{\frac{2ip}{\alpha}(y - y')} \\ &= \left[\sum_m a_m^*(t) \Phi_m^*(x - y) \right] \left[\sum_n a_n(t) \Phi_n(x + y) \right] \end{aligned} \quad (23)$$

So, according to the definition (7) and the expression (11) for the classical probability amplitude, we get

$$T[W](x, y, t) \equiv \int_{-\infty}^{\infty} dp W(x, p, t) e^{\frac{2ipy}{\alpha}} = \Psi^*(x - y, t) \Psi(x + y, t), \quad (24)$$

thus completing the demonstration of the theorem.

3 Considerations concerning the Liouville equation and its connection with the Schrödinger equation

Phase space distribution functions, as those defined in (13), provide a framework for a reformulation of non-relativistic quantum mechanics (QM) in terms of classical concepts [1, 2, 9].

Moreover, it is a widespread belief that the connection between the Liouville equation and the Schrödinger type equation is only possible for quadratic potentials in the x variable ($V(x, t) = a(t)x^2 + b(t)x + c(t)$, where $a(t)$, $b(t)$ and $c(t)$ are arbitrary functions of time [4]). We shall explain, in this section, that the potential energy $V(x)$ can be an arbitrary function of x . In order to achieve this goal we shall use a procedure discussed before by L. S. Olavo [5] and K. Dechoum, H. M. França and C. P. Malta [7]. We shall see that the theorem established in the previous section is a proof of a working hypothesis (see (8)) used in these and many other works [5, 7]. The first work quoted in the reference [7] treats the Stern-Gerlach phenomenon.

As before, $W(x, p, t)$ is the classical phase space probability density associated with some physical system (see the equations (3) and (4)). We shall assume that $W(x, p, t)$ is normalized so that

$$\int dx \int dp W(x, p, t) = 1. \quad (25)$$

The classical configuration space probability density will be denoted by $P(x, t)$ given by

$$P(x, t) = \int dp W(x, p, t) \equiv |\Psi(x, t)|^2. \quad (26)$$

where $\Psi(x, t)$ is the classical probability amplitude (see (6)).

We are interested in obtaining a dynamical differential equation for the classical probability amplitude $\Psi(x, t)$ based on the fact that $W(x, p, t)$ obeys the classical Liouville equation (3).

To obtain this equation, we shall use the Fourier transform

$$T[W](x, y, t) \equiv \int_{-\infty}^{\infty} W(x, p, t) e^{\frac{2ipy}{\alpha}} dp, \quad (27)$$

defined previously in the equation (7).

We recall that the Fourier transform $T[W](x, y, t)$ is a complex function which has a physical meaning only in the limit $|y| \rightarrow 0$, that is,

$$T[W](x, y = 0, t) = |\Psi(x, t)|^2. \quad (28)$$

Therefore, we shall consider the definition (27) only for very small values of y . Our goal is to obtain the differential equation for $\Psi(x, t)$, from the differential equation for $T[W](x, y, t)$, valid when $|y|$ is very small.

Our first step is to consider the equation

$$\frac{\partial}{\partial t} T[W](x, y, t) = \int_{-\infty}^{\infty} \frac{\partial W}{\partial t} e^{\frac{2ipy}{\alpha}} dp. \quad (29)$$

Using the Liouville equation (3) we obtain

$$\frac{\partial T[W]}{\partial t} = - \int_{-\infty}^{\infty} \left[\frac{p}{M} \frac{\partial W}{\partial x} + F(x) \frac{\partial W}{\partial p} \right] e^{\frac{2ipy}{\alpha}} dp. \quad (30)$$

One can show that the integral

$$I = - \int_{-\infty}^{\infty} F(x) \frac{\partial W}{\partial p} e^{\frac{2ipy}{\alpha}} dp$$

is such that

$$I = F(x) \frac{2iy}{\alpha} \int_{-\infty}^{\infty} W(x, p, t) e^{\frac{2ipy}{\alpha}} dp. \quad (31)$$

Here we have assumed that

$$\lim_{|p| \rightarrow \infty} W(x, p, t) = 0. \quad (32)$$

We also see that

$$pe^{\frac{2ipy}{\alpha}} = -i \frac{\alpha}{2} \frac{\partial}{\partial y} e^{\frac{2ipy}{\alpha}}. \quad (33)$$

Substituting (31) and (33) in (30) we get

$$i\alpha \frac{\partial}{\partial t} T[W](x, y, t) = \left[\frac{(-i\alpha)^2}{2M} \frac{\partial^2}{\partial y \partial x} - 2yF(x) \right] T[W](x, y, t). \quad (34)$$

Notice that, in accordance with the theorem proved within section 2, $T[W](x, y, t) = \Psi^*(x - y, t) \Psi(x + y, t)$.

It is convenient to use new variables, namely $s = x - y$ and $r = x + y$, so that the equation (34) can be written as

$$i\alpha \frac{\partial}{\partial t} [\Psi^*(s, t) \Psi(r, t)] = \left[\frac{(-i\alpha)^2}{2M} \left(\frac{\partial^2}{\partial r^2} - \frac{\partial^2}{\partial s^2} \right) - (r - s) F\left(\frac{r + s}{2}\right) \right] \Psi^*(s, t) \Psi(r, t). \quad (35)$$

According to (28), we want an equation for $\Psi(x, t) = [\Psi(r, t)]_{y \rightarrow 0}$, and the equivalent equation for $\Psi^*(x, t) = [\Psi^*(s, t)]_{y \rightarrow 0}$. Consequently we shall consider that the points r and s are arbitrarily close so that

$$-(r - s)F\left(\frac{r + s}{2}\right) = -\int_s^r F(\xi)d\xi = V(r) - V(s), \quad (36)$$

in accordance to the mean value theorem. Substituting (36) into (35) we get the equations

$$i\alpha \frac{\partial}{\partial t} \Psi^*(s, t) = \left[\frac{-1}{2M} \left(-i\alpha \frac{\partial}{\partial s} \right)^2 - V(s) \right] \Psi^*(s, t), \quad (37)$$

and

$$i\alpha \frac{\partial}{\partial t} \Psi(r, t) = \left[\frac{1}{2M} \left(-i\alpha \frac{\partial}{\partial r} \right)^2 + V(r) \right] \Psi(r, t). \quad (38)$$

These two equations are, in fact, the same differential equation, namely

$$i\alpha \frac{\partial}{\partial t} \Psi(x, t) = \left[\frac{1}{2M} \left(-i\alpha \frac{\partial}{\partial x} \right)^2 + V(x) \right] \Psi(x, t), \quad (39)$$

which is formally identical to the Schrödinger wave equation. Notice, however, that $\Psi(x, t)$ is a *classical* probability amplitude, which is conceptually different from the Schrödinger *wave* function $\psi(x, t)$. The classical probability amplitudes $\Psi(x, t)$ are just mathematical objects [16].

The wave-particle duality principle was not used and the small characteristic constant α is, up to this point, arbitrary. This constant can be determined from the observation of several phenomena within microscopic domain [10-12]. Therefore, we can conclude that $\alpha = \hbar$, where \hbar is the universal Planck's constant.

It is relevant to observe that if we write

$$\Psi(x, t) = \Phi_n(x) e^{-i \frac{\epsilon_n t}{\alpha}}, \quad (40)$$

where ϵ_n are constants with dimension of energy, the equation (39) leads to

$$\left[\frac{1}{2M} \left(-i\alpha \frac{\partial}{\partial x} \right)^2 + V(x) \right] \Phi_n(x) = \epsilon_n \Phi_n(x). \quad (41)$$

This is a familiar eigenfunction equation. Its solutions $\Phi_n(x)$ constitute a complete set of orthogonal functions that can be obtained for different potentials $V(x)$. This set of functions $\Phi_n(x)$ can also be used in our previous equations (11) and (13) (see reference [9]) showing the consistency between the sections 2 and 3.

We would like to call the reader attention to the fact that the above mathematical treatment can be extended to the three dimensional case [7] without additional difficulty.

4 Discussion

The connection between the classical Liouville equation for a probability distribution in phase space and the Schrödinger equation was already established for quadratic potentials [1, 4]. The extension of the formalism to a *generic potential* $V(x)$ presented here put all the previous related works [5, 7] on a solid mathematical ground. We get the Schrödinger type equation (39), and also Born's statistic interpretation of $|\Psi(x, t)|^2$, by considering the Liouville equation, and the equations (7), (34) and (35) only in the limit $y \rightarrow 0$. In this context we were able to use the mean value theorem (see equation (36)) to separate (35) in two equivalent equations, formally identical to the Schrödinger equation. Since y has to be small, we understand why the inverse transform (equation (1)), utilized by Wigner, does not guarantee that the phase space function $Q(x, p, t)$ is a true (positive) probability distribution.

The association of the constant α with the Planck's constant \hbar is natural and inevitable to any reader familiarized with the Schrödinger equation used in the microscopic world. As we said above, the explicit numerical value of α (or \hbar) can be determined by testing the validity of the Schrödinger type equation in various phenomena of the microscopic domain [13]. The connection of the Schrödinger momentum operator $-i\hbar\partial/\partial x$ with the zero-point vacuum electromagnetic radiation is also interesting. This fact is explored by P. W. Milonni in the references [14, 15].

According to A. J. Legget [16], “despite the spectacular success of quantum mechanics over the last 80 years in explaining phenomena observed at atomic and subatomic level, the conceptual status of the theory is still a topic of lively controversy”. He seems to believe that quantum mechanics is

nothing more than a very good mathematical “recipe” [17].

We agree with the above statements. According to the connection between the Liouville equation (3) and the Schrödinger type equation (39), presented here, one can conclude that the classical probability amplitude $\Psi(x, t)$ is not associated with a genuine de Broglie wave. As a matter of fact, the existence of de Broglie waves was questioned recently by Sulcs, Gilbert and Osborne [18] in their analysis of the famous experiments [19] on the interference of massive particles as the C_{60} molecules (fullerenes).

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